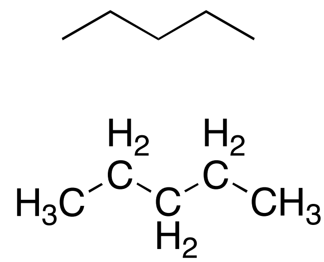
London Forces (temporary dipole):
- also know as dispersion forces
- Principal effect in hydrophobic interaction

Pentane C_5H_{12}

Non-polar molecule

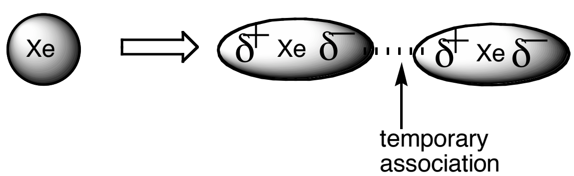
Liquid compared with Methane CH_4 which is a gas



Atoms	boiling point
He	-269 ^{o}C
Ne	-246 ^{o}C
Ar	-186 ^{o}C
Kr	-153 ^{o}C
Xe	-108 ^{o}C

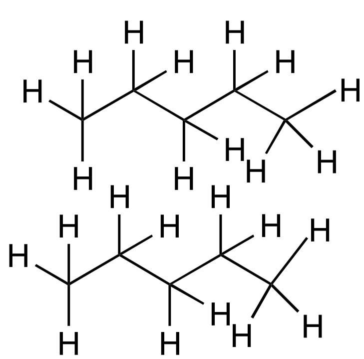
Small atom/ Low polarizability

Large atom/ High polarizability



- the larger the atom (expanded electron density), the easier the formation of temporary dipoles

Hydrophobic interaction: - pentane can develop a similar dipole to that seen for Xe

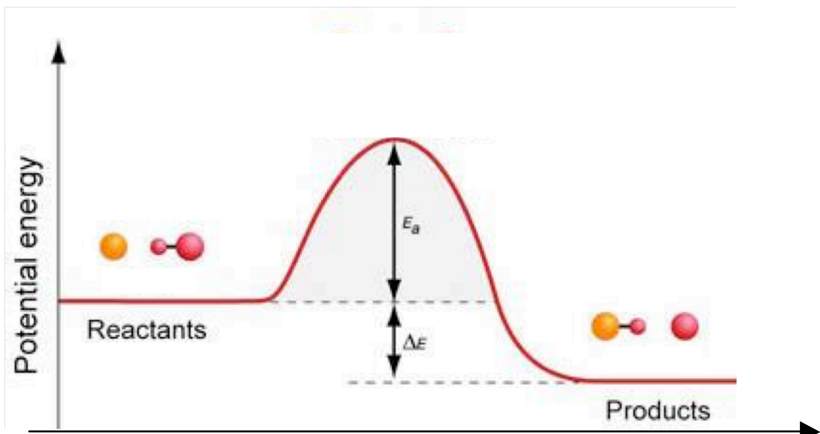


- two pentane molecules have a small attraction to one another at room temperature (hydrophobic interaction)
- This can become a very strong effect with multiple interactions of this type

Reactivity:

$$\underset{\text{(pentane)}}{C_5H_{12}} \quad + \quad \underset{\text{(excess)}}{O_2} \quad \xrightarrow[\text{heat}]{} \quad 5\ CO_2 \quad + \quad 6\ H_2O$$

Energy diagram for reaction



reaction coordinate => progress of reaction

Reactants (starting material): C_5H_{12} and O_2
Products: CO_2 and H_2O

E_a: activation energy
$\Delta E = \Delta G$: Gibbs free energy (enthalpy) change for the reaction
* this reaction is an exothermic reaction, heat is released during reaction

- ΔG = change in energy of system or change in Gibbs free energy.

Temperature in ^oK
($^oK = {}^oC + 273$)

$\Delta G = \Delta H - T\Delta S$ (2nd law of thermodynamics)

Change in enthalpy
= bond energy

Change in entropy
= measure of
disorder in system

$\Delta G = -RT\ln K_{eq}$

R = gas constant = $0.082 \frac{L \cdot atm}{mol \cdot K}$

T = temperature in ^oK

ΔG = change in energy of system (determines equilibrium)

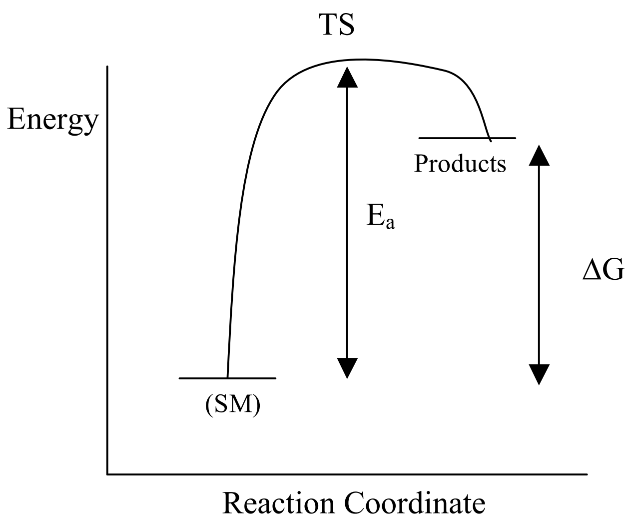
E_a = activation energy → determines rate of reaction

$$A + B \rightleftharpoons C + D$$

K_{eq} = equilibrium constant = $\frac{[C][D]}{[A][B]}$ [C] = concentration of compound C

Endothermic Reaction

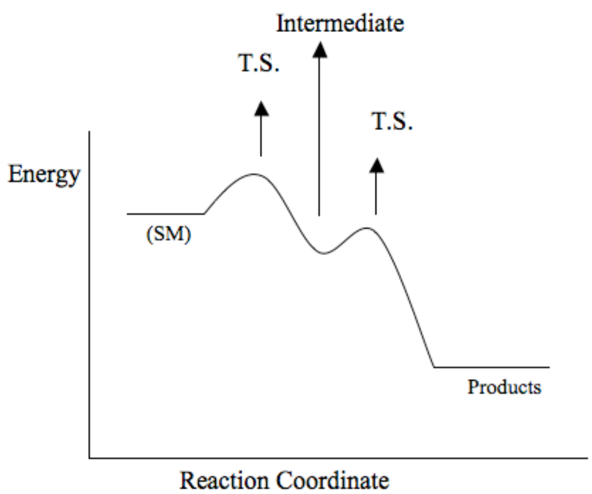
Transition state (TS) = bonds partially made/broken



The transition state is the point of highest energy on the diagram.

The transition state is **not** an intermediate.

Reaction proceeding through an intermediate



Review

$\Delta G = \Delta H - T\Delta S$ (2nd law of thermodynamics)

Change in enthalpy
= bond energy

Exothermic ΔG = Negative

Endothermic ΔG = Positive

Bond Energy

Bond	Bond Energy (kcal/mol)
H-C	99
H-O	111
C-C	83
C=O	179
O=O	119

Ex) $CH_4 + 2\ O_2 \xrightarrow{\Delta} CO_2 + 2\ H_2O$ – Exothermic reaction (releases Energy (E))

$\Delta E_{reaction} = \Delta E_{SM} - \Delta E_{pdt}$

For CH_4:

4 x C-H bonds	= 4 x 99	= 396 kcal/mol	ΔE_{SM} = sum of bonds broken (enthalpy)
2 x O=O	= 2 x 119	= <u>238 kcal/mol</u>	
ΔE_{SM}		= 634 kcal/mol	

For products:

2 C=O	= 2 x 179	= 358 kcal/mol	ΔE_{pdt} = sum of bonds formed
4 H-O	= 4 x 111	= <u>444 kcal/mol</u>	
ΔE_{pdt}		= 802 kcal/mol	

$\Delta E_{reaction}$ = 634 kcal/mol – 802 kcal/mol = -168 kcal/mol (exothermic reaction, energy released)

<u>Acids – Bases</u>

- Bronsted – Lowry
  - An acid donates proton (H^+)
  - A base accepts a proton

Ex

$$HCl \longrightarrow H^+ + Cl^-$$

$$NaOH \longrightarrow Na^+ + OH^-$$

$$HCl + NaOH \longrightarrow NaCl + H\text{-}OH$$

- Lewis
  - An acid accepts a pair of electrons
  - A base donates a pair of electrons

Examples of Lewis acids

H^+ $AlCl_3$ BF_3

Definition

$$H{-}A \rightleftharpoons H^{\oplus} + {:}A^{\ominus}$$

$$K_{eq} = K_a = \frac{[H^+][A^-]}{[HA]}$$

K_a = acidity constant

$pK_a = -\log K_a$

Ex #1)

$$H{-}CH_3 \rightleftharpoons H^+ + CH_3^-$$

$$K_a = \frac{[H^+][CH_3^-]}{[HCH_3]} = 10^{-46}$$

$$pK_a = -\log K_a = 46$$

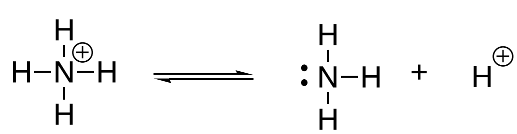
Ex #2)

$$\underset{\text{Ammonia gas}}{H{-}NH_2} \rightleftharpoons H^{\oplus} + {}^{\ominus}{:}\ddot{N}H_2$$

$$K_a = \frac{[H^+][^-NH_2]}{[NH_3]} = 10^{-36}$$

$$pK_a = 36$$

"pKa of Ammonia" in biological system



Ammonium Cation

$pK_a = 9.3$

Ex #3)

$$H{-}O{-}H \rightleftharpoons H^{\oplus} + {}^{\ominus}{:}\ddot{O}H$$

$$K_a = \frac{[H^+][^-OH]}{[HOH]} = 10^{-15.7}$$

$$pK_a = -\log K_a = 15.7$$

Leveling Effect

Strong Acid + Strong Base $\rightleftharpoons$ Weak Acid + Weak Base

Ex)

$$Na^+\ NH_2^- \quad + \quad H\text{-}CH_3 \quad \rightleftharpoons \quad Na^+ :CH_3^- \quad + \quad H\text{-}NH_2$$

Weak Base	Weak Acid	Stronger Base	Stronger Acid

$$NaOH \quad + \quad H\text{-}CH_3 \quad \longleftarrow \quad Na^+ :CH_3^- \quad + \quad H_2O$$

H-CH3: pKa = 46
Weaker Acid

H2O: pKa=16
Stronger Acid

NEXT SECTION : ALKANES

Nomenclature

Learn Names of First 20 Straight Chain Alkanes

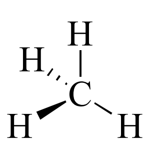
<u>Hydrocarbons</u> – Contain C and H

- Alkanes contain only single bonds (C-H, C-C)
- Alkenes = Olefins C=C
- Alkynes =Acetylenes $C\equiv C$

Alkanes

- All carbons are sp^3 hybridized (bond angle of 109^o)
- Held together by London (dispersion) forces

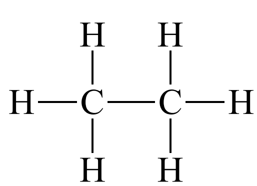
Ex #1) CH_4 , methane



Bp = -161°C

CH_4 H_4C CH_3-H

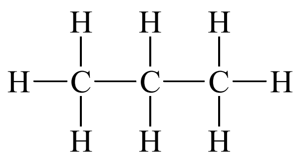
Ex #2) C_2H_6 , ethane



Bp = -88°C

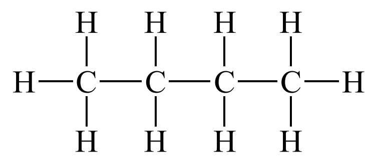
C_2H_6 CH_3-CH_3 H_3C-CH_3

Ex #3) C_3H_8 , propane

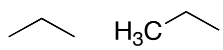


Bp = -42^{o}C

Ex #4) C_4H_{10} , butane



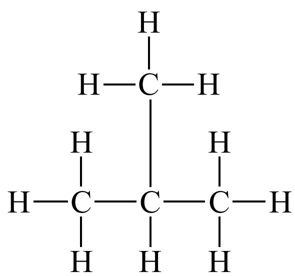
C_3H_8 $CH_3CH_2CH_3$

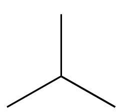


C_4H_{10}, $CH_3CH_2CH_2CH_3$

n-Butane: normal straight chain butane

Ex #5) C_4H_{10} , isobutane





- Isomers (structural or constitutional) are different compounds that have same molecular formula. They have different physical properties (e.g. mp, bp, odour, biological effects)

-	Iso	-	meros
	same	-	parts